# MAGNETIC RESONANCE in CHEMISTRY

1989

Volume 27

MRCHEG 27(1–12)1–1186 (1989)

ISSN 0749–1581

John Wiley & Sons Ltd

# MAGNETIC RESONANCE in CHEMISTRY


**EDITOR-IN-CHIEF**
**Dr P. M. E. LEWIS**
*John Wiley & Sons Ltd, Baffins Lane, Chichester PO19 1UD, UK*

**REGIONAL EDITORS**

**North America**

Professor M. BARFIELD
*Department of Chemistry, University of Arizona, Tucson, Arizona 85721*

Dr S. L. MANATT
*Jet Propulsion Laboratory, Mail Station 183/901, California Institute of Technology, Pasadena, California 91109*

**Europe**

Dr W. BREMSER
*RTL Laboratorium, ROW, Postfach 1464, 5047 Wesseling, West Germany*

Professor G. HABERMEHL
*Chemisches Institut der Tierärztlichen Hochschule Hannover, Bischofsholer Damm 15, 3000 Hannover 1, Germany*

Professor M. L. MARTIN
*Chimie Organique Physique, Université de Nantes, 2 rue de la Houssinière, 44072 Nantes, France*

Professor W. von PHILIPSBORN
*Organisch-Chemisches Institut, Universität Zürich-Irchel, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*

**Australasia**

Professor S. STERNHELL
*Department of Organic Chemistry, University of Sydney, NSW 2006, Australia*

**Asia**

Professor Y. TAKEUCHI
*Department of Chemistry, College of Arts and Sciences, The University of Tokyo, Komaba, Meguro-ku, Tokyo 153*

**USSR**

Professor E. LIPPMAA
*Institute of Chemical Physics and Biophysics, Estonian Academy of Sciences, Lenini Puiestee 10, Tallinn 200001*

Prof. R. J. Abraham
*University of Liverpool*
Dr J. W. Akitt
*University of Leeds*
Prof. F. A. L. Anet
*University of California*
Prof. P. J. Bray
*Brown University, Providence*
Prof. R. G. Bryant
*University of Rochester*
Dr A. M. Chippendale
*ICI plc, Organics Division, Manchester*
Prof. P. Diehl
*University of Basel*
Dr C. M. Dobson
*University of Oxford*
Prof. E. L. Eliel
*University of North Carolina*
Prof. P. D. Ellis
*University of South Carolina*
Prof. S. Fujiwara
*Kanagawa University*
Prof. C. A. Fyfe
*University of Guelph*
Prof. F. Gerson
*University of Basel*
Prof. P. Granger
*Institut de chimie, Strasbourg*
Prof. Dr H. Günther
*University of Siegen*
Prof R. K. Harris
*University of Durham*
Dr H. J. Jakobsen
*University of Aarhus*
Prof. A. R. Katritzky
*University of Florida*
Prof. Dr H. Kessler
*Technische Universität, München, Garching*

**ADVISORY BOARD**

Prof. Dr R. Kosfeld
*Universität Duisberg*
Prof. J. B. Lambert
*Northwestern University, Illinois*
Prof. Dr A. E. Merbach
*Université de Lausanne*
Prof. I. Morishima
*Kyoto University*
Dr G. A. Morris
*University of Manchester*
Prof. M. Ōki
*Okayama University of Science*
Prof. M. Ptak
*Centre de Biophysique Moléculaire, Orléans*
Prof. Dr P. S. Pregosin
*Eidgenössische Technische Hochschule, Zürich*
Prof. W. F. Reynolds
*University of Toronto, Ontario*
Prof. J. D. Roberts
*California Institute of Technology*
Dr J. K. M. Sanders
*University of Cambridge*
Dr J. Schaefer
*Washington University, St. Louis*
Dr J. N. Shoolery
*Varian Associates*
Dr I. C. P. Smith
*National Research Council, Ottawa*
Prof. J. A. S. Smith
*Queen Elizabeth College, London*
Prof. W. B. Smith
*Texas Christian University*
Prof. J. B. Stothers
*University of Western Ontario*
Prof. B. D. Sykes
*University of Alberta*
Prof. F. Taddei
*University of Modena*



Copyright © 1989 by John Wiley & Sons, Ltd.

COPYING OF ARTICLES

The code and the copyright notice appearing at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients, on the condition that the copier pay for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. The per-copy fee for each article appears after the dollar sign, and is to be paid through the Copyright Clearance Center Inc. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Such permission requests, or other inquiries, should be addressed to the publisher.

# Contents of Volume 27

NUMBER 1 JANUARY 1989


**Triazoles. XIV–$^{15}$N NMR Study of Substituted 5-Amino-1,2,4-Triazoles** 1
A. M. ORENDT, J. MICHL AND J. REITER

**$^{1}$H and $^{13}$C NMR Spectral Studies of Some Biquinoline Derivatives and a Re-investigation of the Reaction of Quinoline with Sodium** 4
A. G. OSBORNE, R. GREEN, I. H. SADLER AND D. REED

**$^{1}$H and $^{13}$C Spectra of Fluorine-Containing Polycyclic Aromatic Hydrocarbons. $^{1}$H–$^{19}$F and $^{13}$C–$^{19}$F Coupling Across Bay Regions** 13
D. J. SARDELLA AND E. BOGER

**Application of Data Processing for Sensitivity and Resolution Enhancement of $^{31}$P and $^{13}$C NMR Spectra of Humic Substances** 21
T. KUPKA, J. PACHA AND J. O. DZIĘGIELEWSKI

**Correlation of Carbon-13 Substituent-induced Chemical Shifts Revisited: *meta*- and *para*-Substituted Benzonitriles** 27
O. EXNER AND M. BUDĚŠINSKÝ

**Conformational Analysis via Vicinal Carbon-Hydrogen Coupling** 37
A. L. WATERHOUSE

**The $\gamma$-Butyrolactone Ring Puckering** 44
M. P. GALACHE, P. GARCÉS, A. L. ESTEBAN, E. DIEZ AND J. GUILLEME

**Investigation of Hydrogen-bonded Compounds using High-resolution NMR Spectroscopy in Solids. Part 3—$^{1}$H Chemical Shifts in Polycrystalline Trihydrogen Selenites** 50
H. ROSENBERGER, G. SCHELER AND Yu. N. MOSKVICH

**Investigation of the Behaviour of Propylene Oxide in Water by $^{1}$H NMR Measurements** 57
Y. XUE AND Y.-R. DU

**Rotational Dynamics of Flexible-chain Molecules. $^{13}$C NMR Relaxation Study of Hydrocarbon Chains Attached to a Heavy Anchor** 61
P. DAIS

**DEPT-related Sequences for Selective Long-range Heteronuclear Chemical Shift Correlation Spectroscopy** 68
K. E. KÖVÉR AND Gy. BATTA

**NMR Spectra of Organogermanium Compounds. 8—$^{73}$Ge, $^{13}$C and $^{1}$H NMR Spectra of Methylvinylgermanes** 72
Y. TAKEUCHI, H. INAGAKI, K. TANAKA AND S. YOSHIMURA

**Utility of $^{1}$H/$^{2}$H Isotope Shifts for the $^{13}$C NMR Assignments of Indole Derivatives** 75
M. S. MORALES-RÍOS AND P. JOSEPH-NATHAN

**High-resolution Solid-state $^{119}$Sn and $^{207}$Pb NMR Study of Organotin and Organolead Chalcogenides: Observation of *J*-coupling in Solids** 81
R. K. HARRIS AND A. SEBALD

**$^{14}$N NMR Nuclear Shielding and the Electronic Structure of Dibenzo[1,3a,4,6a]tetrazapentalene** 88
M. WITANOWSKI, J. SITKOWSKI, W. SICIŃSKA, S. BIERNAT AND G. A. WEBB

*Reference Data*

**Carbon-13 NMR Studies of Acridine Derivatives. Part VII.—$^{13}$C Chemical Shifts of Some Substituted 9-Acridanones and 9-Thioacridanones** 92
R. FAURE, J. P. GALY, L. N'GADI AND J. BARBE

**$^{13}$C NMR Structural Analysis of a Series of Tricarbonyl(diene)iron Complexes** 96
J. RODRIGUEZ, P. BRUN, J. P. ZAHRA AND B. WAEGELL

**$^{1}$H NMR Studies on Alkyl-substituted, 2,3- and 3,4-Annulated Tetrahydrothiophenes** 98
R. KIESEWETTER, E. ANKLAM AND P. MARGARETHA

**News and Events, 101; Papers in Press, 102**

NUMBER 2 FEBRUARY 1989

**$^{45}$Sc NMR Study of Scandium Complex Formation in Non-Aqueous Solutions** 103
G. A. KIRAKOSYAN, V. P. TARASOV AND YU. A. BUSLAEV

**High-Resolution $^{1}$H and $^{13}$C NMR Spectroscopy of Some Hydrazo Compounds** 112
J. M. A. AL-RAWI AND M. A. R. KHAYAT

**Proton Nuclear Magnetic Resonance Studies of Dibenzo-*p*-dioxins: Substituent Effects** 117
D. L. ASHLEY, V. VIKRAM REDDY AND D. G. PATTERSON JR.

**Effects of Misoptimization of the BIRD Pulse on One-Bond Modulation Effects in Long-Range Heteronuclear Chemical Shift Correlation Spectra** 123
M. SALAZAR, L. R. SOLTERO, A. S. ZEKTZER AND G. E. MARTIN

**Identification of the b, d, and e Analogs of Vitamin $B_{12}$ as Monocarboxylic Acids by $^{15}$N NMR Spectroscopy** 127
T. J. DIFEO, R. A. SCHIKSNIS, R. K. KOHLI, S. J. OPELLA AND A. NATH

**Reactions of Silver(II) Complexes with Ketoximes, Nitroso and Isonitroso Compounds: ESR Spectroscopy of the Radicals Formed** 130
A. JEZIERSKI

**$^{13}$C NMR Studies of 2- and 3-Methyl- and 2- and 3-Formyl-indoles, Nitro and Phenyl Derivatives** 134
R. ERRA-BALSELLS AND A. R. FRASCA

**$^{1}$H and $^{13}$C NMR Study of the Structure of 3-*N*-(4- and 5-Benzimidazolyl or Benztriazolyl)amino Derivatives of Prop-2-enoic Acid in the Liquid and Solid States** 138
I. GOLJER, V. MILATA AND D. ILAVSKÝ

**Configuration and Solvent-Dependent Conformation of Thiaprotoberberines** 145
P. SOHÁR, L. FODOR, J. SZABÓ AND G. BERNÁTH

**Zwitterionic Piroxicam in Polar Solution** 150
J. M. GECKLE, D. M. RESCEK AND E. B. WHIPPLE

**Definitive Assignment of the $^{13}$C NMR Signals of the Indole C-3 and C-3a Carbons of the Ajmaline Picraline and Sarpagine Alkaloids** 155
M. S. MORALES-RÍOS AND P. JOSEPH-NATHAN

**Experimental and Theoretical Study of the Methoxy Group Conformational Effect on $^{13}$C Chemical Shifts in *ortho*-Substituted Anisoles** 158
R. R. BIEKOFSKY, A. B. POMILIO, R. H. CONTRERAS, D. G. DE KOWALEWSKI AND J. C. FACELLI

**Improved $^{13}$C-$^{1}$H Shift Correlation Spectra for Indirectly Bonded Carbons and Hydrogens; the FLOCK Sequence** 162
W. F. REYNOLDS, S. MCLEAN, M. PERPICK-DUMONT AND R. G. ENRÍQUEZ

**Natural Abundance $^{17}O$ NMR Spectra of Chromanones, Chromones, Flavanones and Flavones** 170
H. DUDDECK, J. C. JÁSZBERÉNYI, A. LÉVAI, T. TIMÁR AND M. H. A. ELGAMAL

**High-Field 2D NMR Spectroscopy of Amanitin Isomers** 173
T. PEHK, M. HAGA, H. VIJA AND E. LIPPMAA

**$^{34}S$ Isotope Effects on $^{31}P$ Chemical Shifts in Thiophosphate Esters** 184
T. BJORHOLM AND F. C. V. LARSSON

**Analysis of the Carbon and Proton NMR Spectra of 2-Arylthiophenes and Related Heterocycles** 187
D. DEL MAZZA, M. G. REINECKE AND W. B. SMITH

**Unusual Behavior of Isopropyl Substituents in 9,10-Dihydroanthracenes: an NMR and Molecular Mechanics Study** 191
P. W. RABIDEAU, W. KIMMER SMITH AND B. D. RAY

*Reference Data*
**The Pyrethrins and Related Compounds 36*—$^{1}H$ and $^{13}C$ NMR Spectra of *cis*- and *trans*-Aryl-Substituted Cyclopentanoid Alcohols and of Their Pyrethroidal Esters** 197
N. F. JANES AND B. P. S. KHAMBAY

**$^{13}C$ NMR Spectra of Antiviral Nucleosides: 3′-Azido-3′-deoxythymidine, 2′,3′-Dideoxyadenosine, 2′,3′-Dideoxycytidine and 2′,3′-Dideoxyinosine** 200
G. W. BUCHANAN AND K. BOURQUE

**$^{13}C$ and $^{1}H$ NMR Chemical Shifts of 2-Substituted Anthracenes** 201
S. BERGER AND B. W. K. DIEHL

**Papers in Press, 204**

NUMBER 3 MARCH 1989

**Phosphorus-Nitrogen Compounds. 59. Aromatic Carbon-13 NMR Spectra of Phenyl-Substituted Cyclotriphosphazatrienes. Second-Order Effects with Phosphorus-31 Nuclei** 207
W. F. DEUTSCH, H. G. PARKES AND R. A. SHAW

**Conjugation of the Cyclopropyl Group** 214
C. GALLI

**$^{1}H$ and $^{13}C$ Dynamic NMR Study of the *E,Z* Isomers of Vinylogous Diamides. Effect of Conjugation and Electrostatic and Steric Repulsion on the C(O)–N Rotation Barriers and Low-Temperature Conformation** 216
G. SZALONTAI, P. SÁNDOR, F. BANGERTER AND L. KOLLÁR

**Nuclear Magnetic Resonance Study of Gentiobiose Octaacetate in Solution** 223
N. MARCHETTINI, S. ULGIATI AND C. ROSSI

**Electron Paramagnetic Resonance Study of the Complex Formed Between Copper and 1-[2(*S*)-3-Mercapto-2-methylpropionyl]-*l*-proline(Captopril) in Solid and Aqueous Solution** 227
J. C. EVANS, C. R. MORRIS, S. B. REES, C. C. ROWLANDS AND D. R. WILLIAMS

**$^{13}C$ NMR Studies on the Structure of Aminosulfonic Acids in Dimethyl Sulfoxide and Water** 233
R. L. BENOIT, D. BOULET AND M. FRÉCHETTE

**NMR Study of Backbone Rearrangements in Gibberellins** 237
A. G. AVENT, J. R. HANSON AND B. H. D'OLIVEIRA

**2-Phenylisatogen: a Study of Molecular Dynamics Using $^{13}C$ NMR Spin-Lattice Relaxation Times** 241
B. STODDART AND M. HOOPER

**$^{1}$H and $^{13}$C NMR Spectra and Rotational Isomerism of 1,3-Dibromobutane** 246
D. W. AKSNES

**Hetero-Association of Caffeine and Theophylline with Purine and Pyrimidine in Aqueous Solutions Studied by $^{1}$H NMR Chemical Shift Measurements** 249
F. ARADI AND A. FÖLDESI

**Two-Bond Deuterium Isotope Effects on $^{13}$C Chemical Shifts. A Measure of Carbon-Carbon Bond Lengths** 253
D. J. SARDELLA AND A. E. EL-DIN

**Expoxidation-Induced Shifts in the Carbon-13 NMR Spectra of Steroids: Lanostane Derivatives** 258
J. MARTYNOW AND Z. PARYZEK

**Principal Component Analysis of the $^{13}$C NMR Shifts of Norbornyl Derivatives** 263
J. G. R. TOSTES, P. R. SEIDL AND R. E. BRUNS

**$^{13}$C Chemical Shift Non-Equivalence in Methylene Carbons of Monosubstituted Cyclohexanes** 273
H. ITO, A. F. RENALDO, R. D. JOHNSON AND M. UEDA

**Intramolecular Non-Bonded Interactions and $^{13}$C NMR Chemical Shifts** 277
R. PACHTER AND P. L. WESSELS

**Aluminium-27 Nuclear Magnetic Resonance Studies of Ferron-Hydroxo-Polynuclear Al Interactions** 283
P. M. BERTSCH, M. A. ANDERSON AND W. J. LAYTON

**Structural Effects on ESR Hyperfine Coupling Constants of Some Dithiazolidinyl Free Radicals** 288
A. M. L. KREBBER, L. H. SUTCLIFFE, W. LUBITZ AND H. KURRECK

**$^{1}$H and $^{13}$C NMR Study of the Interaction of Formaldehyde on Adenine and its Derivatives** 295
D. J. LE BOTLAN

*Reference Data*
**NMR Spectra and Stereochemistry of 1,5- and 1,6-Disubstituted Perhydrooxazolo[3,4-*a*]pyridines** 299
T. A. CRABB AND A. N. TRETHEWEY

**$^{13}$C NMR Chemical Shifts of Substituted 2,2-Dimethyl-2*H*-chromenes** 303
T. TÍMÁR, P. SEBÖK, K. E. KÖVÉR, J. C. JÁSZBERÉNYI AND G. BATTA

NUMBER 4 APRIL 1989

**Studies on Systems of Salts and Mixed Solvents 35-$^{27}$Al NMR Investigations of $AlCl_3$-Water-*N*,*N*-Dimethylformamide Solutions Using the Solid-State MAS Technique** 307
E. HALLAS, H.-H. EMONS, M. SIEDLER AND B. THOMAS

**Solid-state and Solution Conformations of Methadone Hydrochloride and Related Compounds** 311
S. C. J. SUMNER, C. G. MORELAND, F. I. CARROLL, G. A. BRINE AND K. G. BOLDT

**Total Assignment of the $^{1}$H and $^{13}$C NMR Spectra of Phenanthro[9,10-*b*]thiophene: Concerted Use of Two-Dimensional NMR Techniques** 318
M. D. JOHNSTON, JR., M. SALAZAR, L. D. SIMS, A. S. ZEKTZER, R. N. CASTLE AND G. E. MARTIN

**$^{13}$C NMR Studies of Some Tricyclo[3.2.1.$0^{2,4}$]octanes** 323
J. W. WILT, M. PEERAN, S. RAMAKRISHNAN AND D. S. CRUMRINE

**Complexes of Aluminium with Aminopolycarboxylic Acids: $^{27}$Al NMR and Potentiometric Studies** 328
R. K. IYER, S. B. KARWEER AND V. K. JAIN

**Proton NMR Study of Partially Oriented Benzene and Chlorobenzene: Determination of the $r_a$ Structure and of Bond Contributions to the Orientation** 335
R. WASSER, M. KELLERHALS AND P. DIEHL

**Substituent Effects in Cycloheptatrienyl Radicals: an ESR Spectroscopic Study** 340
R. SUSTMANN, D. BRANDES, F. LANGE AND H. I. TASHTOUSH

**$^2$H NMR Study of the Behaviour of Water in a Reversed Micellar System. Hydrogen Bond Breaking and Clathrate Formation by an Inhalation Anaesthetic** 344
A. YOSHINO, T. YOSHIDA AND K. TAKAHASHI

**$^{13}$C NMR Spectral Studies of Some Methoxycoumarin Derivatives. A Re-assignment for Citropten (Limettin) and an Examination of *peri*-Proximity Effects for the Methyl-Methoxy and Methoxy-Methyl Couples** 348
A. G. OSBORNE

**Two-Dimensional NMR Studies of Pt(2-methallyl)($SnCl_3$)(styrene). Recognition and Interpretation of Simultaneous Exchange Processes via $^1$H NOESY** 355
C. AMMANN, P. S. PREGOSIN, H. RÜEGGER, M. GRASSI AND A. MUSCO

**NMR Study of Substituent Effects in 4-Substituted and 4,4′-Disubstituted Diphenyl Sulphoxides and Sulphones** 360
R. CHANDRASEKARAN, S. PERUMAL AND D. A. WILSON

**NMR Study of the Monomer-Dimer Equilibria of Dimethylnitrosobenzenes in Solution. Identification of Mixed Azodioxy Dimeric Species** 368
K. G. ORRELL, D. STEPHENSON AND T. RAULT

**$^{71}$Ga Nuclear Magnetic Resonance Investigation of Aqueous Gallium(III) and its Hydrolysis** 377
J. W. AKITT AND D. KETTLE

**Effects of Solute-Solvent Interactions on the Nitrogen Nuclear Shieldings of Some Alkyl Cyanides** 380
M. WITANOWSKI, W. SICINSKA AND G. A. WEBB

**Nuclear Spin Relaxation of Oxygen-17, Silicon-29 and Carbon-13 in Octamethylcyclotetrasiloxane** 386
J. KOWALEWSKI AND E. BERGGREN

**NMR Spectra and Conformational Analysis of Substituted 1,3,4,5-Tetrahydro-2*H*-1,5-benzodiazepin-2-one Derivatives** 391
F. MALIK, M. HASSAN, D. ROSENBAUM AND H. DUDDECK

*Short Communication*
**2D Heteronuclear NOE Spectroscopy with Full $\Omega_1$ Decoupling. A Method for Elimination of $^{13}$C-$^1$H Coupling Dependence** 396
K. E. KÖVÉR AND GY. BATTA

*Reference Data*
**$^{13}$C NMR Study of *ortho*-, *meta*- and *para*-Alkoxycarbonylalkyloxychalcones and Their $\alpha,\beta$-Dibromo Derivatives** 399
M. SZAJDA

**Analysis of the $^1$H NMR Spectra of the Carboxylic Ionophore Narasin A in its Apo and Cation-Bound Forms** 403
B. W. CAUGHEY, W. A. GIBBONS AND G. R. PAINTER

**Book Review, 407; Papers in Press, 408**

NUMBER 5 MAY 1989

**Review**

**Effect of Electron Lone-Pairs on Nuclear Spin–Spin Coupling Constants** 409
V. M. S. GIL AND W. VON PHILIPSBORN

**Chemistry of the S═O Bond. 11.Carbon-13 and Oxygen-17 Nuclear Magnetic Resonance Studies on Stereoisomerism in 1,3,2-Dioxathiepanes** 431
D. G. HELLIER AND H. G. LIDDY

**Two-Dimensional NMR Spectroscopy of LL-F28249-$\alpha$, a Potent Macrolide Anthelmintic: $^{13}C$, $^{1}H$ Chemical Shift Assignments and Solution Conformation** 437
S. RAJAN AND G. W. STOCKTON

**$^{1}H$ NMR Studies of Proton Transfer in *ortho*-Mannich Bases** 445
M. ROSPENK AND L. SOBCZYK

**Involvement of Exciplexes in the Photolysis of Aliphatic Ketones in Deuteriochloroform: CIDNP Evidence** 451
M.-X. ZHANG, Z.-L. LIU, L.-M. WU AND Y.-C. LIU

**Observation of a Tight-Turn Conformation in a Proline-Containing Inhibitor of Renin Angiotensin** 455
S. SRIVASTAVA, R. S. PHADKE AND G. GOVIL

**$^{13}C$ NMR Spectroscopy of Aristolochic Acids and Aristololactams** 460
H. A. PRIESTAP

**Solid-State NMR Study of a Series of Aminophosphonic Acids** 470
R. K. HARRIS, L. H. MERWIN AND G. HÄGELE

**Complete $^{1}H$ and $^{13}C$ NMR Assignment of Two $\alpha$-Isosparteine Salts by the Use of Two-Dimensional NMR Spectroscopy** 476
M. F. SIMEONOV, S. L. SPASSOV, H. DUDDECK, U. MAJCHRZAK-KUCZYŃSKA AND J. SKOLIK

**Lanthanide-Induced Shifts in the $^{1}H$ NMR Spectra of *N,N*-Dimethylformamide and *N,N*-Dimethylacetamide: Limitations of the Point Methyl Model** 483
J. A. LADD

**Molecular Conformation Trapping as an Aid to Chemical Shift Assignments for Multi-Conformation Systems: a Platinum (II) Complex** 488
L. A. LUCK, W. L. ELCESSER, J. L. HUBBARD AND C. H. BUSHWELLER

**Transfer of Polarization in the Rotating Frame. Application to Drug-Nucleotide Complexes** 491
J. BELLENEY AND M. DELEPIERRE

*Reference Data*

**Proton Nuclear Magnetic Resonance Study of the Biologically Active Peptide Analog [Pro$^{2}$]-Thymopentin** 496
G. K. GRIFFITH, D.-H. HUANG, D. G. NETTESHEIM, G. A. HEAVNER AND N. R. KRISHNA

**$^{1}H$ and $^{13}C$ Chemical Shifts of Some 1,2-Dithiole-3-Thione Derivatives** 498
C. VACCHER, P. BERTHELOT AND M. DEBAERT

**Tellurium-125 NMR Investigations on Coordination Compounds of Tellurium(II) with Unsaturated Dithio, Thioseleno and Diseleno Ligands** 500
W. DIETZSCH, R.-M. OLK, E. HOYER, W. MEILER AND W. ROBIEN

**$^{1}H$ and $^{13}C$ NMR Studies on Mono- and Polybrominated Biphenyls** 503
E. ANKLAM

**Book Reviews, 507; Announcements, 509; Papers in Press, 510**

**Inter- and Intra-molecular Hydrogen Bonding Effects on Geminal $^{15}N$, $^{1}H$ Spin Coupling and $^{15}N$ Chemical Shifts in Pyridine Derivatives** 511
W. HOLZER AND W. VON PHILIPSBORN

**Quantitative Small Molecule NOESY. A Practical Guide for Derivation of Cross-relaxation Rates and Internuclear Distances** 515
N. H. ANDERSEN, H. L. EATON AND X. LAI

**Establishing Long-Range Connectivities in Polynuclear Aromatics Through the Use of Two-Dimensional MLEV-17-Based Isotropic Mixing** 529
M. D. JOHNSTON, JR., AND G. E. MARTIN

**Simple Model for NMR Relaxation Times of Flexible Molecules in Solution** 533
M. BALDO AND A. GRASSI

**$^{13}C$ NMR Studies of *cis-trans* Isomerization of *N*-Benzylidene-Propyl- and -Substituted Aryl-Amines Induced by a Lanthanide Shift Reagent** 540
J. M. A. AL-RAWI AND L. M. N. SALEEM

**$^{13}C$ and $^{1}H$ NMR Investigations of Quinic Acid Derivatives: Complete Spectral Assignment and Elucidation of Preferred Conformations** 544
A. FLORES-PARRA, D. M. GUTIÉRREZ-AVELLA, R. CONTRERAS AND F. KHUONG-HUU

**Relationship Between Proton-Proton NMR Coupling Constants and Substituent Electronegativities. IV—An Extended Karplus Equation Accounting for Interactions Between Substituents and its Application to Coupling Constant Data Calculated by the Extended Hückel Method** 556
L. A. DONDERS, F. A. A. DE LEEUW AND C. ALTONA

**Relationship Between Proton-Proton NMR Coupling Constants and Substituent Electronegativities. V—Empirical Substituent Constants Deduced from Ethanes and Propanes** 564
C. ALTONA, J. H. IPPEL, A. J. A. WESTRA HOEKZEMA, C. ERKELENS, M. GROESBEEK AND L. A. DONDERS

**$^{13}C$ NMR Study of the Substituent Effects on the Internal Steric Hindrances in Amidines** 577
I. WAWER

**Quantitative Analysis and Determination of the Enantiomeric Purity of Glycerides by $^{13}C$ NMR Spectroscopy. Application to the Lipase-Catalysed Transesterification of Triacylglycerides** 582
C. RABILLER AND F. MAZE

**Correlation of Carbon-13 Substituent-Induced Chemical Shifts: *meta*- and *para*-Substituted Methyl Benzoates** 585
M. BUDĚŠÍNSKÝ AND O. EXNER

**Effect of Methylation on the Association Ability of Purine and Pyrimidine in Aqueous Solutions. A $^{1}H$ NMR Chemical Shift Study** 592
F. ARADI AND A. FÖLDESI

*Short Communication*
**Carbon-Phosphorus Heteronuclear Shift Correlation via Multiple Quantum Coherence** 599
L. D. SIMS, L. R. SOLTERO AND G. E. MARTIN

*Reference Data*
**NMR Studies in the Heterocyclic Series. XXXII. Carbon-13 NMR Study of *N*-Arylpyrazoles and *N*-Arylpyrazolium Salts** 603
A. DE LA HOZ, M. DEL CARMEN PARDO, J. ELGUERO AND A. FRUCHIER

**Linear and Angular Effects on the $^{1}H$ and $^{13}C$ NMR Spectra of Tricyclic Aromatic Ketones Formally Derived from Tetralone** 606
G. W. BUCHANAN, P. T. TONG, R. H. WIGHTMAN AND B. A. DAWSON

**Carbon-13 NMR of the *N*-Substituents in 2,4,6-Trisubstituted Pyridinium Salts** 608
S. R. SALMAN AND M. A. R. KHAYAT

NUMBER 7 JULY 1989

**Quantitative Evaluation of Electronic Effects of the 1-Tetrazolyl Group from $^{1}H$ and $^{13}C$ NMR Data for Substituted 1-Phenyltetrazoles** 611
V. P. KARAVAI, P. N. GAPONIK AND O. A. IVASHKEVICH

**$^{13}C$ and $^{1}H$ NMR Studies of Some Aminoarsonium Chlorides** 616
C. L. WATKINS, L. K. KRANNICH, R. K. KANJOLIA AND D. K. SRIVASTAVA

**Different Solution and Solid-state Conformations of the Antibiotic Cycloheximide** 624
N. B. PERRY, J. W. BLUNT AND M. H. G. MUNRO

**$^{6}Li$ *J*-Modulated $^{13}C$ Spin-echo Spectra. Selective Observation of Alkyllithium Aggregates** 628
R. D. THOMAS AND D. H. ELLINGTON

**NMR Spectral Assignment and Conformation of Macrocyclic Biaryl Ethers from *Garuga Gamblei*** 635
H. KALCHHAUSER AND H. G. KRISHNAMURTY

**Assignments of Phosphate Groups and Determination of P,H Coupling Constants in the DNA Fragment d(CGTACG) by $^{31}P$ 2D NMR Experiments** 640
E. RAGG, R. MONDELLI, A. GARBESI, F. P. COLONNA, C. BATTISTINI AND S. VIOGLIO

**$^{13}C$ Nuclear Magnetic Resonance Study of Some Phosphinolipids: Assignments and Conformational Studies** 647
G. KALLINOWSKI AND W. VOGT

**$^{13}C$ NMR of Coumarins. II – Khellactones: Spectroscopic Criteria to Establish the Relative Configuration of the Dihydropyran Ring** 653
F. A. MACÍAS, G. M . MASSANET, F. RODRÍGUEZ-LUIS, J. SALVÁ AND F. R. FRONCZEK

**Utilization of the Selective Pulse INEPT NMR Experiment (INAPT) for the Facile Distinction of Quaternary Carbons Attached to a Trisubstituted Alkene** 659
M. A. BERNSTEIN

**Effect of Substituents on the $^{13}C$ NMR Chemical Shifts of 2-R-3-Methylbenzothiazolium Quaternary Salts and 2-R-Benzothiazoles** 663
E. SOLČÁNIOVÁ AND I. ČULÁK

**Determination of the $^{13}C$ Chemical Shift Tensors in Isotactic Polypropylene via the Two-dimensional Powder Pattern in Rotating Solids** 666
T. NAKAI, J. ASHIDA AND T. TERAO

**Two-dimensional NMR Studies of Arsenical-Sulfhydryl Adducts** 669
R. J. O'CONNOR, E. L. McGOWN, K. DILL AND S. F. HALLOWELL

**The Stereochemistry of Crown Ethers. III – Conformational Variations During Alkali Complexation** 676
E. KLEINPETER, S. STOSS, M. GÄBLER AND W. SCHROTH

**Proton and Carbon NMR Spectra of 2-Substituted Dibenzothiophenes** 684
S. JAYALAKSHMI, S. PERUMAL AND D. A. WILSON

**2-(4′-Substituted)-phenylisatogens: Analysis of $^{13}C$ Substituent Chemical Shifts** 687
B. STODDART AND M. HOOPER

**Solid-state $^{13}C$ Chemical Shift Calculations in Aryl Ether Compounds** 692
N. J. CLAYDEN

**Partial Editing in Heteronuclear *J*-Resolved Solid-state NMR Spectroscopy** 696
P. TEKELY, J. BRONDEAU, A. RETOURNARD AND D. CANET

**Short Communication**
**Unprecedented Example of a $^3J(^{13}C,^{11}B)$ Through a C-C-N-B Linkage** 699
J. ATCHEKZAÏ, B. BONNETOT, J.-C. DUPLAN, B. FENET, B. FRANGE AND H. MONGEOT

**Reference Data**
**$^{13}C$ NMR Study of Tetrahydrothiazolo[3,2-*d*][1,4]benzodiazepin-3(2*H*)-ones** 702
M. ZAPPALÀ, G. ROMEO, S. GRASSO, A. CHIMIRRI AND A. M. MONFORTE

**$^{13}C$ NMR of Coumarins I: 3-(1,1-Dimethylallyl) Derivatives** 705
F. A. MACÍAS, G. M. MASSANET, F. RODRÍGUEZ-LUIS AND J. SALVÁ

**Assignment of $^1H$ and $^{13}C$ NMR Spectra of Retinoic Acid Ester Isomers Observed in the Long-Wavelength UV-Induced Photostationary State** 707
R. W. CURLEY, JR. AND J. W. FOWBLE

**Book Review, 710; Papers in Press, 711**

NUMBER 8 AUGUST 1989

**Dynamic NMR Study of the Electronic State of Heteroaromatics. V – Influence of the Counter Anion, *ortho* Substituents and the Ring Heteroatom on the Exocyclic C,N Rotational Barrier of Pyrylium and Thiopyrylium Salts** 713
E. KLEINPETER, R. SPITZNER AND W. SCHROTH

**Reaction of Dibenzalcyclohexanone with Hydroxylamine Hydrochloride. 2D NMR Elucidation of the Structure of the Products** 719
E. DÍAZ, H. BARRIOS, B. ORTIZ, R. SÁNCHEZ-OBREGÓN, F. YUSTE, W. F. REYNOLDS, J. L. AGUILERA AND E. CABALLERO

**Studies on the Benzoxazine Series 2 – Preparation and $^1H$ and $^{13}C$ NMR Structural Study of Some Substituted 1,2-Dihydro-4*H*-3,1-benzoxazines** 725
K. NEUVONEN, R. POHTOLA AND K. PIHLAJA

**NMR Shift Reagents for Organic Salts: Shift Mechanism, Bound Shifts and Structural Analysis** 734
T. J. WENZEL AND K. CAMERON

**Full Assignments of the $^1H$ and $^{13}C$ NMR Spectra of Sodium Fusidate in Organic and Aqueous Media** 740
J. BARBER, L. LIAN, G. A. MORRIS AND M. H. TEHRANI

**Full Assignments of the $^1H$ and $^{13}C$ NMR Spectra of the Antibiotic Kirromycin (Mocimycin)** 748
J. BARBER, A. E. DEROME, T. D. HOWARD, L. LIAN AND G. TEBB

**Determination of the Pyrrolizidine Alkaloids from *Senecio jacobaea* by $^1H$ and $^{13}C$ NMR Spectroscopy** 754
L. A. C. PIETERS, A. M. VAN ZOELEN, K. VRIELING AND A. J. VLIETINCK

**Synthesis and Conformational Analysis of Dibenzodithiocin Derivatives** 760
P. SOHÁR, I. KÖVESDI, J. SZABÓ, Á. KATÓCS, L. FODOR, E. SZÜCS, G. BERNÁTH AND J. TAMÁS

**$^{13}C$ and $^1H$ NMR Study of Structure and Structural Dynamics of Tautomeric 2-Ethoxycarbonylthiolane-3-thiones** 767
F. DUUS

**EPR Study of Radicals Derived from Fumaronitrile and Related Carboxylic Acids** 782
P. SMITH, W. H. DONOVAN AND J. K. PARKER

**Complete Assignment of the $^{13}C$ and $^{1}H$ NMR Spectra of Thyrsiferyl Acetate** 792
J. W. BLUNT, J. D. McCOMBS, M. H. G. MUNRO AND F. N. THOMAS

**Revised Assignments of the $^{13}C$ NMR Spectra of Some Hydrophenanthrenes** 796
L. ERNST AND R. STOLLE

**NMR Spectroscopy of Paramagnetic Complexes. Part 36 – $^{2/1}H$ NMR of Paramagnetic Metallocenes: Primary and Secondary Isotope Effects and Signal Narrowing** 798
N. HEBENDANZ, F. H. KÖHLER, F. SCHERBAUM AND B. SCHLESINGER

**Reference Data**
**$^{1}H$ and $^{13}C$ NMR Analysis of Three Quinone-Methide Triterpenoids** 803
A. A. L. GUNATILAKA, H. C. FERNANDO, T. KIKUCHI AND Y. TEZUKA

**$^{13}C$ Chemical Shift Assignments for Isomers of Some 1,2-Diaroyl-3-arylcyclopropanes** 807
D. B. REDDY, B. V. REDDY, T. SESHAMMA, B. SANKARAIAH AND M. V. R. REDDY

**Complete Assignment of the $^{1}H$ and $^{13}C$ NMR Spectra of 1,3-Diaza-2,4-diboranaphthalene Derivatives by Two-dimensional NMR Spectroscopy** 809
S. ALLAOUD, H. BITAR, B. FRANGE AND R. FAURE

**Book Review, 812; Papers in Press, 813**

NUMBER 9 SEPTEMBER 1989

**Structure of and Electronic Interactions in Aromatic Polyvalent Iodine Compounds: a $^{13}C$ NMR Study** 815
A. R. KATRITZKY, J. K. GALLOS AND H. DUPONT DURST

**Reaction of Dibenzalacetone with Hydroxylamine Hydrochloride Under Phase-Transfer Conditions. $^{1}H$ and $^{13}C$ 2D NMR Structural Elucidation of the Products** 823
J. L. AGUILERA, G. SOSA, W. F. REYNOLDS, E. DIAZ AND H. BARRIOS

**Natural Abundance Carbon-13 and Deuterium NMR Studies on the Liquid and Solid Phases of *tert*-Butyl Iodide** 830
D. W. AKSNES AND K. RAMSTAD

**Study of Hydrolytic Kinetics of the Hexachlorostannate Anion by Two-Dimensional $^{119}Sn$ Exchange Spectroscopy** 836
X.-A. MAO, X.-Z. YOU AND A.-B. DAI

**$^{13}C$ NMR Spectra of Some Halocarbons. Shift Predictions in Polychloro-quinolines and -isoquinolines** 841
R. S. MATTHEWS, M. JONES AND J. BANKS

**ESR Evidence for the Stereospecific Spin Trapping of 5-Alkyl-5-methyl-1-pyrroline *N*-oxides** 846
Y. ZHANG AND G. XU

**$^{13}C$ NMR Studies of Insulin Part I — Spectral Assignments** 852
D. J. CRAIK, K. A. HIGGINS, J. G. HALL AND P. R. ANDREWS

**Complete $^{1}H$ and $^{13}C$ NMR Spectral Assignment of Venturicidin A by 2D NMR Spectroscopy** 863
A. GOGOLL AND D. TANNER

**Structure of Norbornene-Fused 3,1-Oxazine Double Cycloadducts** 872
P. SOHÁR, G. BERNÁTH, G. STÁJER AND A. E. SZABÓ

**Proton-Detected C,H Correlation NMR Techniques for the Complete Assignment of all Proton and Carbon Resonances of a Cyclic Peptide** 877
M. HOFMANN, M. GEHRKE, W. BERMEL AND H. KESSLER

**EPR and ENDOR Study of Chiral Nitroxides** 887
H. B. STEGMANN, F.-M. SCHABER, P. SCHULER AND K. SCHEFFLER

**Reference Data**

**$^{13}$C NMR of Coumarins III – Simple Coumarins** 892
F. A. MACIAS, G. M. MASSANET, F. RODRÍGUEZ-LUIS AND J. SALVÁ

**$^{13}$C Relaxation in Cyclopentadienyliron Dicarbonyl Acyl Compounds** 895
L. E. NANCE, H. J. WILL, D. BRENT MacQUEEN, J. M. GARRISON AND J. M. NICKLAW

**$^{13}$C NMR Spectra of Amino-alkylphosphonic Acids** 897
Z. GŁOWACKI AND M. TOPOLSKI

**$^{1}$H and $^{13}$C NMR Spectra of 4,4′-Substituted Chalcones** 899
K. HAYAMIZU, M. YANAGISAWA, T. ISHII, A. YABE, O. YAMAMOTO, M. NAKAYAMA AND A. HAYASHI

**Book Review, 905; Papers in Press, 905**

NUMBER 10 OCTOBER 1989

**Relationships Between $^{1}$H, $^{13}$C and $^{17}$O NMR Chemical Shifts and H/D Isotope Effects on $^{13}$C and $^{17}$O Nuclear Shielding in Intramolecular Hydrogen-Bonded Systems** 907
E. LIEPIŅŠ, M. V. PETROVA, E. GUDRINIECE, J. PAULIŅŠ AND S. L. KUZNETSOV

**Dynamic Nuclear Magnetic Resonance Study of Intramolecular Processes in Cyclohexanediaminetetraacetate—Metal Complexes** 916
Y. BA, R.-F. SONG AND Z.-W. QIU

**$^{31}$P NMR Enantiomeric Purity Determination of Free 1-Aminoalkylphosphonic Acids via Their Diastereoisomeric Pd(II) Complexes** 922
Z. GŁOWACKI, M. TOPOLSKI, E. MATCZAK-JON AND M. HOFFMANN

**Assignment of the $^{1}$H, $^{13}$C and $^{15}$N NMR Spectra of Methyl *β-D*-Glucopyranoside Tetranitrate, *β*-Cellobiose Octanitrate and Cellulose Trinitrate by Two-dimensional Homonuclear and Heteronuclear $^{13}$C–$^{1}$H and $^{15}$N–O–C–$^{1}$H Shift Correlation Spectroscopy** 925
T. AXENROD, B. LIANG AND S. BULUSU

**NMR Study of Three Heteroyohimbine Derivatives from *Rauwolfia Serpentina*: Stereochemical Aspects of the Two Isomers of Reserpiline Hydrochloride** 935
A. DE BRUYN, W. ZHANG AND M. BUDĚŠÍNSKÝ

**Carbon-13 Chemical Shielding Tensors in Alkanedicarboxylic Acids. Influence of Molecular Geometry on the Carboxyl Carbon Tensors in Alkanedicarboxylic Acids and Related Compounds** 941
N. R. JAGANNATHAN

**Assigned Cluster $^{11}$B and $^{1}$H NMR Properties of [3-($\eta^6$-$C_6Me_6$)-*closo*-3,1,2-$RuC_2B_9H_{11}$]** 947
M. BOWN, J. PLEŠEK, K. BAŠE, B. ŠTÍBR, X. L. R. FONTAINE, N. N. GREENWOOD AND J. D. KENNEDY

**Interpretation of the Solvent Effect on the Screening Constant of Xe-129** 950
M. LUHMER, A. DEJAEGERE AND J. REISSE

**The Influence of Crown Ethers on Cation Migration Processes. Part 7. The 2-Pivaloyl-1,4-benzoquinone Radical Anion** 953
N. J. FLINT AND B. J. TABNER

**Preparation and Structure of Cycloalkane-Condensed [1,3]Thiazino[3,2-*a*] pyrimidinones** 959
P. SOHÁR, Z. SZÖKE-MOLNÁR, G. STÁJER AND G. BERNÁTH

**Stereochemical Studies of the 4-Alkyl-4-Arylpiperidine Class of Opioid Ligand** 964
A. F. CASY, G. H. DEWAR AND O. A. A. AL-DEEB

**High Resolution NMR Study of Some Chromium Compounds in Solution** 973
M. F. A. DOVE, E. M. Ll. JONES AND R. J. CLARK (in part)

**A $^{1}$H and $^{13}$C NMR Study of *N*-Formylmorphinans and Their 6,14-Bridged Derivatives; Comparison with *N*-Me and *N*-H Analogues** 980
J. T. M. LINDERS, M. A. PRAZERES, T. S. LIE AND L. MAAT

**$^{1}$H and $^{13}$C NMR Study of the Adsorption of Alcohols on Charcoals with Various Pore Structures** 987
Y.-R. DU, H.-Z. YUAN, D.-H. WU AND Y.-H. KONG

**Short Communication**

**$^{13}$C NMR Studies of Tautomerism in Imidazo[4,5-*c*]pyridines** 992
P. BARRACLOUGH, J. C. LINDON, M. S. NOBBS AND J. M. WILLIAMS

**Reference Data**

**$^{1}$H, $^{13}$C 2D NMR Experiments for the Identification of an Impurity in Lauryl Lactam from Cyclododecane** 995
J.-P. HUVENNE, B. LAMY AND B. MOUCHEL

**Two-dimensional NMR Study of Ganwuweizic Acid** 998
Y.-X. CUI, S.-M. HUA, J.-L. CHENG, J.-M. YUE AND Y.-Z. CHEN

**Assignments of the $^{1}$H and $^{13}$C NMR Resonances of C-Nucleoside Analogues by Means of Two-Dimensional Shift Correlated NMR Techniques** 1001
F. DENNIN, O. ROUSSEAUX, D. BLONDEAU AND H. SLIWA

**Book Reviews, 1004; Press Release, 1005; Papers in Press, 1006**

NUMBER 11 NOVEMBER 1989

**$^{13}$C NMR Study of 2-Iodoso- and 2-Iodoxy-benzoic Acids and Their Sodium Salts** 1007
A. R. KATRITZKY, B. L. DUELL, J. K. GALLOS AND H. D. DURST

**$^{1}$H and $^{13}$C NMR Assignments for Lanostan-3$\beta$-ol Derivatives: Revised Assignments for Lanosterol** 1012
G. T. EMMONS, W. K. WILSON AND G. J. SCHROEPFER, JR

**Pseudolaric Acid B: NMR Assignments, Conformational Analysis and Cytotoxicity** 1025
M. O. HAMBURGER, H.-L. SHIEH, B.-N. ZHOU, J. M. PEZZUTO AND G. A. CORDELL

**Solvent Effect on the $^{13}$C and $^{15}$N NMR Chemical Shifts and Rotational Barriers in *N*,$^{1}$*N*$^{1}$-Dimethyl- and *N*,$^{1}$*N*$^{1}$-Hexamethylene-*N*$^{2}$-Phenylformamidines** 1031
I. WAWER

**Isotope Effects on the $^{13}$C NMR Chemical Shifts of 5-Substituted Indoles: Evidence for Electron Density Dependence on the Hydrogen (Deuterium) Atom** 1039
M. S. MORALES-RÍOS, R. E. DEL RÍO AND P. JOSEPH-NATHAN

**$^{13}$C NMR Assignment of Protonated Carbons in d-type Porphyrins** 1048
R. TIMKOVICH AND L. L. BONDOC

**Measurement of Long-Range Proton-Carbon Coupling Constants in Medium-Sized Molecules** 1052
M. HRICOVÍNI AND T. LIPTAJ

**Complete Spectral Assignments of Tatsidine by Two-dimensional NMR Techniques** 1057
J. K. SNYDER, B. S. JOSHI, X. ZHANG AND S. W. PELLETIER

**Exceptional Resolution and New Signals Detected in the $^{13}$C NMR Spectra of Alkanes** 1065
L. B. ALEMANY

**Substituent Chemical Shifts in NMR. Part 4—$^{1}$H SCS in Some 2-Substituted Norbornanes and Bornanes** 1074
R. J. ABRAHAM, A. P. BARLOW AND A. E. ROWAN

**Short Communication**

**Suppression of Artefacts in Nuclear Overhauser Effect Difference Spectroscopy by Reference Deconvolution** 1085
G. A. MORRIS AND D. COWBURN

**Reference Data**

**Proton and Carbon-13 NMR Studies of 1-Substituted Pyridinium Salts** 1090
A. R. KATRITZKY AND Z. DEGA-SZAFRAN

**Two-dimensional NMR Analysis of Selected Benzazolo[3,2-*a*]quinolinium Salts** 1094
O. COX, J. A. PRIETO AND M. RODRIGUEZ

**Proton and Carbon-13 NMR Study of Scopoline and its Derivatives** 1097
P. SCHEIBER AND K. NÁDOR

**Natural Abundance One-Bond $^{13}$C-$^{13}$C Coupling Constants and Unambiguous Assignments of $^{13}$C NMR Spectra of Thieno[*c*]quinolines and Thieno[*c*]isoquinolines** 1099
S. GRONOWITZ, R. SERVIN AND Y. YANG

**$^{1}$H and $^{13}$C NMR Studies of Some *O*-Carbamoyloximes** 1102
M. I. M. WAZEER, SK. A. ALI AND M. ARAB

**$^{13}$C NMR Spectra of Some 4-Substituted *N*-Acetonyl-*N*,*N*-dimethyl-*N*-phenacyl-ammonium Bromides** 1104
J. GRANDJEAN, P. LASZLO, E. L. DO CANTO AND R. RITTNER

**Papers in Press, 1106**

NUMBER 12 DECEMBER 1989

**Probing the Mechanism of Ligand Exchange by Two-Dimensional NMR Spectroscopy** 1107
M. J. HAMPDEN-SMITH AND H. RUEGGER

**$^{29}$Si and $^{13}$C NMR Spectra of Alkenyl- and Alkynyl-trimethylsilanes** 1112
M. I. AL-HASSAN, I. M. AL-NAJJAR AND I. M. AL-ORAIFY

**$^{59}$Co NMR of Cobalt(III) Porphyrin Complexes. III. Data Base on Substituent and Solvent Effects** 1117
H. BANG, L. CASSIDEI, H. DANFORD, J. O. EDWARDS, K. I. HAGEN, C. KRUEGER, J. LACHOWITZ, C. M. SCHWAB, D. A. SWEIGART AND Z. ZHANG

**$^{13}$C NMR Study of Substituted 10,10-Diphenyl-9-Phenanthrones. Structure Determination and Signal Assignment using 2D NMR Techniques** 1130
R. MYNOTT, M. J. ROMÃO AND B. J. HEROLD

**Accuracy of Molecular Dynamics Obtained by $T_{1\rho}$ Measurements on the Microsecond Time Scale in Solution** 1134
Y.-S. WANG AND S. IKUTA

**$^{1}$H and $^{13}$C NMR Studies on the Oxydimethyleneaminomethyl Fragment in Six- and Eight-Membered Rings. The Solution Stereochemistry of *N*-Methyl Diastereomers of Phendimetrazine (an Oxazine Anorexic Drug) *versus* Nefopam (a Benzoxazocine Analgesic Drug)** 1142
R. GLASER

**NMR Self-diffusion Measurements: A Different Approach to Complexation Phenomena** 1148
M. GERINGER AND H. STERK

**Revised $^{13}$C NMR Signal Assignments of 2-(Bromomethyl)naphthalene** 1155
L. ERNST

**Single-Crystal Electron-Spin Resonance Study of the 4-Phenyl-1,2,3,5-dithiadiazolyl Radical** 1161
F. L. LEE, K. F. PRESTON, A. J. WILLIAMS, L. H. SUTCLIFFE, A. J. BANISTER AND S. T. WAIT

**$^{13}$C NMR Data for Isopimarane and 8-*epi*-Isopimarane Diterpenoids** 1166
A. SAN FELICIANO, M. MEDARDE, F. TOMÉ, B. HEBRERO AND E. CABALLERO

**Reference Data**

**$^{13}$C NMR of Lapachol and Some Related Naphthoquinones** 1176
B. A. DAWSON, M. GIRARD, D. KINDACK, J. FILLION AND D. V. C. AWANG

**$^{13}$C NMR Chemical Shifts of the Carbon Atoms of the Methoxymethyl Group of Di-*ortho*-substituted Aromatic Methoxymethyl Ethers** 1178
T. S. KAUFMAN, R. D. SINDELAR AND A. R. JÜRGENS

**Carbon-13 NMR Chemical Shift Assignment of Neoflavonoids** 1180
G. D. MONACHE, I. MESSANA, B. BOTTA AND E. GÁCS-BAITZ

**Forthcoming Meetings, 1184; Papers in Press, 1186; Author Index, i**